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9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NL 110 Duncan Ave Room B115 Bolling AFB DC 20332-8050  Dr Michael R. Berman		10. SPONSORING / MONITORING AGENCY REPORT NUMBER
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13. ABSTRACT (Minimum 200 words)

The focus of the research program supported by this grant is the formulation, development, implementation and application of modeling strategies and large-scale computer simulation methods for studies of critical issues in two main areas: (i) Tribological Interactions, Nanomechanics, Thin Film Lubrication, and dynamical and rheological properties of thin films of complex molecular liquids. (ii) Surface processing, the stability of nanostructures on surfaces, and the mechanical and electric properties of interfacial junctions. (iii) Structure, dynamics, and thermodynamics of nanocrystals and their two and three-dimensional assemblies. Significant progress has been achieved in both the aforementioned main areas of research, as well as in related areas. These achievements include: (ii) Investigations of: the dynamics of superheating, melting, and annealing processes of metallic surfaces under intense irradiation; surface premelting of metal surfaces; stability and collapse mechanisms of metallic nanostructures on surfaces; the mechanical and electric properties of interfacial solid junctions (nanowires), including conductance quantization and localization phenomena; surface crystallization, dynamics of evaporation and condensation, and segregation phenomena in liquid n-alkane films;

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molecular dynamics, flow and rheology in thin-film lubricated junctions, sheared at ultra-high velocities, and including effects due surface morphological inhomogeneities, phase coexistence in finite material aggregates (large metal and ionic clusters); collective excitations in nanostructures; structure, energetics, dynamics, assembly mechanisms, and thermodynamics of nanocrystals (bare and passivated) and their assemblies.

Final Report

AFOSR Grant F49620-93-1-0231

Microscopic Modeling of Nanotribology Lubrication and Wear,

Surface Processing and Nanostructures

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## 1. Objectives

The focus of the research program supported by this grant is the formulation, development, implementation and application of modeling strategies and large-scale computer simulation methods for studies of critical issues in two main areas:

- (i) Tribological Interactions, Nanomechanics, Thin Film Lubrication, and dynamical and rheological properties of thin films of complex molecular liquids.
- (ii) Surface processing, the stability of nanostructures on surfaces, and the mechanical and electric properties of interfacial junctions.
- (iii) Structure, dynamics, and thermodynamics of nanocrystals and their two and three-dimensional assemblies.

The program serves as a focus for investigations in materials science and computational methodologies regionally, nationally and internationally. Several of our projects are performed in collaboration with experimental laboratories (e.g., investigation of nanocluster assemblies and conductance in nanowires). In addition to the scientific goals the program fulfills educational ones through the training of post-doctoral fellows (currently one from Paris, supported through independent resources, i.e., the French science foundations), and graduate students (currently two Ph.D. thesis students at GA Tech).

During the current report period the main research efforts were aimed toward the above objectives, coinciding with the objectives listed in the Research Proposal underlying this program.

## 2. Status

Significant progress has been achieved in both the aforementioned main areas of research,

as well as in related areas. These achievements include:

(i) Development of computer codes for large-scale simulations of complex physical systems allowing realistic simulations of their properties. Such systems include: metal surfaces described via many-body interactions and under the influence of intense laser irradiation, as well as thermal heating; interfaces between solid surfaces and organic liquids (particularly paraffines used as model lubricants); non-uniform interfacial junctions lubricated by confined complex fluids, allowing investigations of atomic-scale mechanisms of thin-film viscous elastohydrodynamic lubrication.

(ii) Investigations of: the dynamics of superheating, melting, and annealing processes of metallic surfaces under intense irradiation; surface premelting of metal surfaces; stability and collapse mechanisms of metallic nanostructures on surfaces; the mechanical and electric properties of interfacial solid junctions (nanowires), including conductance quantization and localization phenomena; surface crystallization, dynamics of evaporation and condensation, and segregation phenomena in liquid n-alkane films; molecular dynamics, flow and rheology in thin-film lubricated junctions, sheared at ultra-high velocities, and including effects due surface morphological inhomogeneities; phase coexistence in finite material aggregates (large metal and ionic clusters); collective excitations in nanostructures; structure, energetics, dynamics, assembly mechanisms, and thermodynamics of nanocrystals (bare and passivated) and their assemblies.

The above developments in simulation methodology and investigations of the properties of materials with refined atomic-scale resolution, open new avenues for preparation, fundamental understanding and utilization of complex materials in advanced technologies, such as ultra high-density magnetic information storage and retrieval (thin-film boundary lubricated), high-

performance engines, electronic device miniaturization, and surface processing and damage annealing via heating. In the following we summarize some of the major accomplishments of our research.

### 3. Accomplishments/New Findings

#### (i) **Mechanical and Electric Conductance Properties of Metallic Nanowires**

Material systems of reduced size or dimensionality may, and often do, exhibit properties different from those found in the bulk. These include quantized conductance in point contacts and narrow channels whose characteristic (transverse) dimensions approach the electronic wavelength, localization phenomena in low-dimensional systems, and mechanical properties characterized by a reduced propensity for the creation and propagation of dislocations in small metallic samples. Such phenomena are of considerable scientific and technological interest, particularly in the area of miniaturized, highly compact, electronic devices.

We reported (Science 267, 1793 (1995), and J. Vac. Sci. Technol. B 13, 1280 (1995)) on investigations of the evolution of room-temperature electronic transport properties in Au nanowires, from quantized conductance [in  $2e^2/h$  or  $2(2e^2/h)$  steps, where  $h$  is Planck's constant] with a spatial periodicity of  $\sim 2 \text{ \AA}$  during elongation of short ( $\sim 50 \text{ \AA}$ ) wires, to the onset of localization in long ( $100 \text{ \AA} < \ell < 400 \text{ \AA}$ ) ones. Combining electronic conductance measurements with molecular dynamics (MD) simulations of the wire elongation process reveals that for short wires, the periodic occurrence of quantized conductance, accompanied by characteristic "dips" [local conductance minima associated with the presence of disorder], is correlated with atomic-scale structural transformations that occur during the layer-by-layer order-disorder elongation

process. The dominance of disorder and the onset of localization in long wires (longer than the localization length) are exhibited by a nonlinear dependence of the resistance  $R$  on the length of the wire  $\ell$  as it is pulled continuously [that is,  $\ln R(\ell) \sim \ell^2$ ]. Moreover, current versus voltage data, recorded at selected stages in the elongation process, indicate gradual loss of metallic character as the long wire narrows.

Junctions and materials structures which form upon bringing bodies into proximal interaction, during the separation of contacting bodies, in the process of extension (e.g., pulling) of a material system, or in the course of growth (e.g., fabrication of thin film junctions). Past, as well as intensifying current, investigations of junctions have been motivated by the ubiquity of circumstances in which they may be formed; either naturally in the course of a physical process (as in the case of materials interfaces in relative motion with respect to each other where the frictional resistance to shear has been attributed to the formation of interfacial junctions, or as the source of interfacial adhesive action) or intentionally (e.g., controlled generation of wires via the extension of materials contacts, as in the case of surface manipulations using tip-based methods, a break-junction technique, or by separation of wires in contact).

Our early investigations (Science 248, 454 (1990)) were the first to predict the formation of nanowires, elucidate their generation mechanisms and mechanical response, and anticipate their unique electronic transport properties. More recently, we have discovered the effects of shape and magnetic fields on the nature of electronic conductance, culminating in our prediction of a novel magnetic switching of quantum transport through nanowires (Phys. Rev. B 53, 13246 (1996), Rapid Communication), which is subsequently being investigated experimentally in several laboratories.

Furthermore, in a recent study (Phys. Rev. Lett. 77, 1362 (1996)) we have investigated the electrical conductance and principal structural and mechanical properties of gold nanowires, exhibiting reversibility in elongation-compression cycles at ambient conditions, using pin-plate experiments and molecular dynamics simulations. We have discovered that underlying the reversible nature of the nanowires are their crystalline ordered structure and their atomistic structural transformation mechanisms, involving stages of stress accumulation and stress relief occurring through multiple-glide processes and characterized by a high critical yield stress value.

These investigations open exciting new avenues for further studies and potential applications such as switching and miniaturized machine elements.

#### **(ii) Nano-Elastohydrodynamic Thin-Film Lubrication**

The major development in the understanding of fluid film lubrication which has taken place during the second half of the 20th century was enabled by the recognition of the beneficial influence of both elastic deformations of the solids and the increase in viscosity of the lubricant with pressure in highly stressed lubricated machine elements. The consequent development of elastohydrodynamic lubrication (EHL) theory, and micro-EHL, allowed the design of machine elements and bio-tribological systems of improved efficiency and durability.

Certain current novel technologies (such as high density information storage and retrieval systems, and high performance engines), and those projected for the next century, present new tribological challenges due to the miniaturization of devices operating under extreme conditions. Motivated by such considerations, and by the recent emergence and proliferation of new experimental proximal probes allowing high resolution controlled measurements, our present



theoretical investigations aim at providing insights into the atomic-scale fundamental processes of ultra thin-film lubrication, thus extending EHL into the nano-realm.

Atomic-scale structure, dynamics, flow and response characteristics of a thin film molecular hexadecane lubricant, confined and sheared by topographically nonuniform solid gold surfaces which slide at a relative velocity of 10 m/s, were investigated using molecular dynamics simulations.

Our findings (Science 270, 605 (1995) and Langmuir 12, 4514 (1996)) pertaining to molecular ordering, layering processes in lubricants confined and sheared at high velocities by topographically non-uniform solid surfaces and their correlation with oscillatory patterns in the friction force, lubricant-mediated structural transformations and modifications of the solid surfaces, dynamical formation of elastoplastic states of the lubricant due to extreme confinement between the sliding asperities, and the appearance of post-asperity-collision nano-scale cavitated zones, go beyond the predictions of continuum theories and provide the impetus for future experimental and theoretical investigations. Our current investigations include systems under various loads and different shearing velocities, lubrication under constant load conditions, thermal effects, three dimensional asperities, multi-asperity contacts, homogeneous lubricants of various chain lengths and molecular architectures, studies of lubricant mixtures, and lubricant degradation as well as tribochemical processes.

A major review by U. Landman (written together with two leading experimentalists) has been written and published in Nature 374, 607 (1995), titled "Nanotribology: Friction, Wear and Lubrication at the Atomic Scale".

### **(iii) Size-Evolutionary Patterns and Nanocrystals**

Characterization and elucidation of size-evolutionary patterns of the properties of finite materials aggregates exhibiting discrete quantized energy level spectra and specific structures and morphologies, investigations of unique properties of finite-size materials clusters, and studies of the nature of the evolution from the molecular and cluster regimes to the bulk phase are among the major challenges of modern materials science and have been the subject of intensive research endeavors. These investigations, which include explorations of structural, electronic, thermodynamic, spectroscopic, and chemical properties of isolated clusters and their assemblies, have revealed unique size-dependent physical and chemical materials phenomena differing from those found in the bulk, motivating some to classify such materials aggregates of reduced dimensions as a distinct state of matter. Furthermore, nanophase materials built through the assembly of nanometer-scale units into ordered superlattices offer exciting perspectives as novel materials whose optical, electronic, and transport properties may be controlled by the selection of the composition and sizes of the building-block units, suggesting their potential utilization as components in electronic, optoelectronic, and sensor technologies.

The creation of perfect single crystallites, identically replicated in unlimited quantities, in a state that can be handled, manipulated, treated and understood, is an ultimate challenge of modern materials science with outstanding fundamental and potential technological consequences. Combined theoretical and experimental efforts aimed at the synthesis, processing, isolation and characterization of monodispersed nanocrystalline gold assemblies resulted in a significant advance in this area of research (Adv. Mater. 8, 428 (1996)). The theoretical studies revealed that the optimal structures of gold nanocrystals in the range of a few tenths to thousands of gold

atoms, belong to a definite structural motif, consisting of finite fcc lattices with a truncated octahedral (and variants thereof) morphology. These theoretical predictions were verified by experiments (mass spectrometry, high-resolution electron microscopy, and x-ray diffraction) on fractionated samples of gold nanocrystals, passivated by self-assembled monolayers, which have been isolated as distinct, pure molecular materials of high intrinsic stability.

The structure, dynamics, and thermodynamics of gold nanocrystallites passivated by alkylthiolate monolayers were investigated for the first time, using molecular dynamics simulations, in different environments - as isolated gas-phase clusters, when adsorbed on a graphite surface, and when assembled into three-dimensional superlattices (J. Phys. Chem. 100, 13323 (1996)). Here we summarize the main findings of these studies. The packing arrangements and densities of the monolayers passivating the facets of the core gold nanocrystallites differ from those found on extended gold surfaces, exhibiting organization into molecular bundles of preferred orientations which upon heating undergo a reversible melting transition from the ordered bundled state to a uniform intermolecular orientational distribution. The equilibrium geometries of adsorbed nanocrystallites depend on the chain length of the passivating molecules which effectively lubricate the interface between the gold core and the graphite surface conferring high surface mobility to the crystallites, involving a collective slip-diffusion mechanism. The room-temperature equilibrium structure of the superlattice made of  $\text{Au}_{140}(\text{C}_{12}\text{H}_{25}\text{S})_{62}$  nanocrystallites is predicted to be tetragonally distorted fcc with enhanced orientational bundling of the passivating molecules along the direction of the tetragonal distortion. The cohesion of the superlattice derives dominantly from the interactions between the interlocking molecular bundles. On the other hand, passivation by shorter chain molecules,  $\text{Au}_{140}(\text{C}_4\text{H}_9\text{S})_{62}$ ,

results in a room-temperature body-centered cubic superlattice structure, transforming to a fcc lattice at higher temperatures.

**(iv) Superheating, Melting and Annealing of Metallic Surfaces, and the Stability of Metallic Structures on Surfaces**

Methods of processing of materials surfaces via laser irradiation are of fundamental as well as technological and economic significance, since various physical and chemical surface properties (such as optical and electrical characteristics, corrosion resistance, composition, morphology, and structure) can be influenced and/or modified using such methods in a controlled and spatially selective manner. Furthermore, with the use of short laser pulses, detailed time-resolved experimental investigations of electron-phonon energy transfer mechanisms and relaxation times, and of the thermal and structural evolution of metal surfaces (disordering, melting, and most recently superheating of the Pb(111) surface, have been performed.

We reported (Phys. Rev. Lett. 71, 1023 (1993), and App. Surf. Sci. 92, 237 (1996)), on molecular dynamics simulations of laser irradiation of copper surfaces, which differ from continuum treatments of such phenomena and previous simulations by explicitly including the temporal laser excitation of the electrons and their coupling to the microscopic dynamics of the nuclear degrees of freedom which are modeled using realistic interactions. Our simulations demonstrate that under irradiation conditions for which the Cu(110), as well as Cu(100), surfaces undergo melting, superheating of perfect as well as damaged Cu(111) occurs, in correspondence with recent experiments. Moreover, under the same conditions, a damaged Cu(111) surface (containing initially a large vacancy cluster and an adlayer island) superheats and anneals,

restoring perfect crystalline order, via a nondiffusional mechanism involving local incorporation (embedding) of adlayer atoms and subsequent cooperative displacements of the host surface layer atoms to fill the vacancy region. This finding is of particular relevance in light of the experimental observations, where the sample surfaces are most likely to contain, even under equilibrium conditions, a certain fraction of spontaneously generated defects which could serve as nucleation centers for melting, and is related to the energetics of the (111) surface.

Basic and technological interest in the physical properties of small materials structures, and in locally controlled surface modifications, underlie intensifying research endeavors in this area. Using molecular dynamics (MD) simulations, we have explored the structure, energetics, dynamics, stability, and collapse mechanisms of surface-supported metallic nanostructures which are key issues in preparation, control, and exploitation of such structures (Phys. Rev. Lett. 73, 569 (1994)).

We showed that heterostructures, such as a three-dimensional (3D) crystalline gold cluster (dot) deposited on a Ni(100) surface, where the lattice mismatch is large (16%) and the surface energy of the nickel substrate is larger than that of the deposited Au dot, can collapse via a nondiffusional solid-on-solid settling (SOSS) mechanism. The SOSS process involves a succession of layer-by-layer incorporations (embedment) of Au atoms from a given layer into the underlying Au layer, accompanied by subsequent cooperative stress relief via lateral displacements of atoms in the underlayer. These processes result ultimately in transformation of the initial 3D structure into a 2D adsorbed gold island whose area grows linearly with time. On the other hand a homostructure, e.g., a 3D crystalline gold cluster deposited on an Au(111) surface, adsorbs epitaxially (in registry) with the substrate, exhibits enhanced stability and collapses at elevated

temperatures via a dislocation mediated settling (DMS) mechanism, involving vacancies generated by surface dislocations in the deposited Au cluster. These novel atomic-scale mass transport and collapse mechanisms and the interplay between interfacial energetics and structure which they portray, pertain to a number of interfacial processes (e.g., deposited nanostructures, thin-film growth, annealing of damage, surface manipulations, and nanoscale lithography).

#### 4. Personnel

##### Supported by Grant:

Uzi Landman - Callaway Chair in Computational Materials Science and Regents' Professor

W. D. Luedtke - Senior Research Scientist

C. Yannouleas - Research Scientist

H. Hakkinen - Post-Doctoral Fellow (until October 1994).

E. Ringer - Graduate Student

##### Associated with the Research Effort:

T. K. Xia - Research Scientist

C. L. Cleveland - Senior Research Scientist

J. Ouyang - Graduate Student (received Ph.D. degree in 1994)

E. N. Bogachek - Senior Research Scientist

#### 5. Publications

1. "Molecular Dynamics of Adsorption and Segregation from an Alkane Mixture", T. K. Xia and U. Landman, *Science* **261**, 1310 (1993).
2. "Superheating, Melting and Annealing of Copper Surfaces", H. Hakkinen and U. Landman, *Phys. Rev. Lett.* **71**, 1023 (1993).
3. "Structure and Dynamics of Surface Crystallization of Liquid n-Alkanes", T. K. Xia and U. Landman, *Phys. Rev. B* **48**, 11313 (1993).
4. "Interfacial Junctions and Cavitation", U. Landman and W. D. Luedtke, an invited paper in *Mater. Res. Bulletin* **18**, (May), 36 (1993).
5. "Phase Coexistence in Clusters", C. L. Cleveland, U. Landman, and W. D. Luedtke, *J. Phys.*

- Chem. 98, 6272 (1994).
6. "Stability and Collapse Mechanisms of Adsorbed Metallic Structures", U. Landman and W. D. Luedtke, Phys. Rev. Lett. 73, 569 (1994).
  7. "Molecular Evaporation and Condensation of Liquid n-Alkane Films", U. Landman and T. K. Xia, J. Chem. Phys. 101, 2498 (1994).
  8. "Properties of Metallic Nanowires: From Conductance Quantization to Localization", J. I. Pascual, J. Mendez, J. Gomez-Herrero, A. M. Baro, N. Garcia, U. Landman, W. D. Luedtke, E. N. Bogachek and H.-P. Cheng, Science 267, 1783 (1995).
  9. "Electrical and Mechanical Properties of Metallic Nanowires: Conductance Quantization and Localization", J. I. Pascual, J. Mendez, J. Gomez-Herrero, A. M. Baro, U. Landman, N. Garcia, W. D. Luedtke, E. N. Bogachek and H.-P. Cheng, J. Vac. Sci. Technol. B 13(3) 1280 (1995).
  10. "Equilibrium Interphase-Interfaces and Premelting of the Pb(110) Surface", A. Landa, P. Wynblatt, H. Hakkinen, R. N. Barnett, and U. Landman, Phys. Rev. B 51, 10972 (1995).
  11. "Molecular Dynamics Study of Disordering and Premelting of the Pb(110) Surface", A. Landa, H. Hakkinen, R. N. Barnett, U. Landman, and P. Wynblatt, (in press, MRS, 1995).
  12. "Nanotribology: Mechanisms and Consequences", B. Bushan, J. Israelachvili, and U. Landman, Nature 374, 607 (1995).
  13. "Nano-Elastohydrodynamics: Structure, Dynamics and Flow in Nonuniform Lubricated Junctions", J. Gao, W. D. Luedtke and U. Landman, Science 270, 605 (1995).
  14. "Atomistic Dynamics of Interfacial Processes: Films, Junctions and Nanostructures", U. Landman and W. D. Luedtke, Appl. Surf. Sci. 92, 237 (1996).



15. "Barriers and Deformation in Fission of Metal Clusters", C. Yannouleas and U. Landman,  
J. Phys. Chem. 99, 14577 (1995).
16. "Collective Excitations of Multishell Carbon Superstructures: Multishell Fullerenes  
and Coaxial Nanotubes", C. Yannouleas, E. N. Bogachek, and U. Landman, Phys. Rev. B  
53, 10225 (1996).
17. "Atomic Scale Issues in Tribology: Interfacial Junctions and Nano-Elastohydrodynamics",  
U. Landman, J. Gao and W. D. Luedtke, Langmuir 12, 4514 (1996).
18. "Quantum Electronic Transport Through Three-Dimensional Microconstrictions With  
Variable Shapes", A. G. Scherbakov, E. N. Bogachek, and U. Landman Phys. Rev. B 53,  
4054 (1996).
19. "Atomistic Dynamics of Interfacial Processes: Films, Junctions and Nanostructures",  
U. Landman and W. D. Luedtke, Appl. Surf. Sci. 92, 237 (1996).
20. "Nano-Crystal Gold Molecules", U. Landman, W. L. Whetten, J. Khoury, I. Vezmar,  
S. Murthy, C. L. Cleveland, W. D. Luedtke, Adv. Mater. 8, 428 (1996).
21. "Magnetic Switching and Thermal Enhancement of Quantum Transport Through  
Nanowires", E. N. Bogachek, A. G. Scherbakov, and U. Landman, Phys. Rev. B 53 R  
13246 (1996).
22. "Reversible Manipulations of Room Temperature Mechanical and Quantum Transport  
Properties in Nanowire Junctions", U. Landman, W. D. Luedtke, B. E. Salisbury, and R. L.  
Whetten, Phys. Rev. Lett. 77, 1362 (1996).
23. "Water Adsorption and Reactions on Small Sodium-Chloride Clusters", R. N. Barnett

- and U. Landman, J. Phys. Chem. 100, 13950 (1996).
24. "Thermopower of Quantum Nanowires in a Magnetic Field", E. N. Bogachek, A. G. Scherbakov, and U. Landman, Phys. Rev. B 54, R11094 (1996).
25. "Structure, Dynamics, and Thermodynamics of Passivated Gold Nanocrystallites and Their Assemblies", W. D. Luedtke and U. Landman, J. Phys. Chem. 32, 13323(1996).
26. "Molecular Dynamics Study of Disordering, Roughening, and Premelting of the Pb(110) Surface", A. Landa, H. Hakkinen, R. N. Barnett, P. Wynblatt, and U. Landman, J. Non-Cryst. Solids 205, 767 (1996).

#### Book Chapters

1. "Consequences of Tip-Substrate Interactions", U. Landman and W. D. Luedtke, in "Scanning Microscopy III, eds. R. Wiesendanger and H.-J. Guntherodt, in press (Springer, Berlin, 1993), p. 207.
2. "Simulations of Materials: Clusters and Interfacial Junctions", in "Computations for the Nanoscale", U. Landman, R. N. Barnett, H.-P. Cheng, C. L. Cleveland, and W. D. Luedtke, eds. P. E. Blochl, A. J. Fisher, and C. Joachim, (Kluwer, Dordrecht, 1993), p. 75.
3. "Nanocrystal Gold Molecules", with R. L. Whetten et al., in "The Chemical Physics of Fullerenes 10 (and 5) Years Later", W. Andreioni, ed. (Kluwer, Dordrecht, 1996), p. 475.
4. "Nano-Elastohydrodynamics", U. Landman, J. Gao and W. D. Luedtke, in "Physics of Sliding Friction", B. J. Persson and E. Tossati, eds. (Kluwer, Dordrecht, 1996), p. 325.
5. "Junctions and Nano-Elastohydrodynamics", U. Landman, W. D. Luedtke and J. Gao, in "Micro/Nanotribology and its Application", Ed. B. Bhushan (Kluwer, Dordrecht, 1997),

p. 493.

## 6. Interactions/Transitions

### (a) Invited Talks

- Keynote Speaker at 4th European Conference on Surface Crystallography, Aarhus, Denmark, May, 1993.
- Invited Speaker, European Research Conference on "Fundamentals of Clusters", Crete, Greece, May, 1993.
- Plenary Speaker at "Physics Computing 1993", Albuquerque, N. M., June, 1993.
- Invited Speaker at International Conference on "Theory of Atomic and Molecular Clusters I", LEER, Germany, July, 1993.
- Invited Speaker at Gordon Conference on "Gas Surface Dynamics", August, 1993.
- Invited Speaker and Discussion Leader, Gordon Conference on "Metal and Semiconducting Clusters", NH, August, 1993.
- Invited Speaker and Session Chairman at CCP5 Conference on "Large Scale Molecular Simulations", Keele, England, September, 1993.
- Invited Speaker at Workshop on "From Microscopics to Macroscopics", Yorktown Heights, October, 1993.
- Invited Speaker at Workshop on "Future Direction in Molecular Physics", Max-Planck Institute, Gottingen, Germany, December, 1993.
- Invited Speaker, MRS Meeting, Boston, December, 1993.
- Invited Speaker in "Physics of Confined Layers", LesHouches, France, February, 1994.
- Invited Lecturer in NATO Advanced Study Institute on "Atomic Force Microscopy", Schlussee, Black Forest, Germany, March, 1994.
- Invited Speaker, APS Meeting, Pittsburgh, PA, March, 1994.
- Invited Speaker, ACS Meeting, San Diego, CA, March, 1994.
- Invited Speaker, US-Japan Seminar on "Frontiers in Clusters", Hawaii, March, 1994.
- Invited Speaker, NATO Advanced Study Institute on "Atomic Force Microscopy of Organic Layers", Schloss-Ringberg, Germany, June, 1994.
- Invited Speaker, European Physics Conference on "Electronic Structure and Excitation in Solids", Gausdal, Norway, August, 1994.
- Invited Speaker, Unilever Royal Society UK-Indo Forum on "Solid-Solid Interactions", London, September, 1994.
- Invited Speaker, International Symposium on "Molecular Dynamics", Minneapolis, Minnesota, October, 1994.
- Invited Speaker, European Research Conference on "Fission Phenomena", Treno, Italy, October, 1994.
- Invited Speaker, "International Conference on Surfaces and Thin Films, ICSFS-7", Hsinchu, Taiwan, December, 1994.

Invited Speaker, MRS Meeting, Boston, December 1994.  
Invited Speaker, AAAS Annual Meeting, Atlanta, Georgia, January, 1995.  
American Physical Meeting (8 talks), San Jose, CA, March, 1995.  
Invited Speaker, American Chemical Society, Anaheim, CA, April, 1995.  
Invited Speaker, American Association of Black Physicists, Atlanta, GA, April, 1995.  
Invited Speaker, NATO Advanced Study Institute, International School of Solid State Physics, 6th Course, "Large Clusters of Atoms and Molecules", E. Majornan Centr for Scientific Culture, Erice, Italy, June, 1995.  
Invited Speaker, International Conference on "Physics of Sliding Friction", International Center for Theoretical Physics, Trieste, Italy, June, 1995.  
Invited Speaker, International Conference on "Computational Methods in Materials Science and Engineering", International Center for Theoretical Physics, Trieste, Italy, June, 1995.  
Invited Speaker, Gordon Conference on "Metal and Semiconductor Clusters", New Hampshire, August, 1995.  
Invited Speaker, "Tribology Workshop", Orono, Maine, August, 1995.  
Keynote Speaker, CCP5 Annual Meeting, "Advanced Computer Simulations of Materials", Daresbury, England, September, 1995.  
Keynote Speaker, International Conference on Clusters, Barcelona, Spain, September, 1995.  
Invited Speaker, 3rd International Symposium on Atomically Controlled Surfaces and Interfaces, Raleigh, N. C., October, 1995.  
Invited Speaker, International Conference on "Atomistically Controlled Surfaces and Interfaces", (ACSI-3), N. C. State, Raleigh, Oct., 1995.  
Invited Speaker, "Sanibel Symposium" St. Augustine, FL, Feb. 1996.  
Invited Speaker, APS Meeting, St. Louis, March 1996.  
Invited Lodestar Lecture, 1996 ASME Mechanics and Materials Conference, Baltimore, MD, June 1996  
Invited Lecturer, "Nato Advanced Study Institute Course on Micro/Nanotribology and its Applications", Villas de Sesimbra, Portugal, June 1996.  
Invited Speaker, "International Symposium on Small Particles and Inorganic Clusters", Copenhagen, July 1996.  
Invited Speaker, "Cluster Interactions with Surfaces", Rostock, Germany, July 1996.  
Invited Speaker, ACS Meeting, Orlando, FL, August, 1996.  
Invited Speaker, Nato Advanced Workshop on "Nanowires", Sept. 1996.  
Plenary Lecture in "Quantum Optics and Clusters", Joint Polish-German Conference, Katowica, Poland, September, 1996.  
Invited Speaker, American Vacuum Society Annual Meeting, Philadelphia, Oct. 1996.  
Invited Speaker, "Friction, Arching, Contact Dynamics", Julich, Germany, Oct. 1996.  
Invited Speaker, MRS Annual Meeting, Boston, Nov. 1996.

(b) Several of our research findings were reviewed and/or highlighted by popular science magazines, industrial, engineering, and R&D journals and news releases, and by the media. These include:

- Science News.
- Advanced Materials and Processing (June, 1995), p. 4.
- Industry Week (May 1, 1995), p. 46.
- Materials Research Society Bulletin (May, 1995).
- Inside R&D Magazine, (April 12, 1995).
- Appearance by U. Landman on the "Quirks and Quarks" program, broadcasted by the Canadian Broadcasting System, in February 1995.

#### 7. Honors and Professional Appointments

- (i) Appointment of U. Landman in 1994 to the Editorial Board of "Tribology International".
- (ii) Appointment of U. Landman in 1994 to the Editorial Board of the Journal of Physical Chemistry.
- (iii) U. Landman was appointed in January 1995 as the Fuller E. Callaway Professor in Computational Materials Science, at the Georgia Institute of Technology.
- (iv) U. Landman has been selected as one of the "50 Stars of the Year" by "Industry Weekly", December 18 issue.
- (v) U. Landman's invited lecture on nanocrystals and nanowires, at the Annual APS Meeting (St. Louis, March, 1996) has been listed and described in the June 1996 issue of APS News as one of twelve highlights (out of about 4,200 technical papers) of the meeting.

(vi) U. Landman delivered an invited Lodestar Lecture, titled, "Materials by Numbers", at the ASME Mechanics and Materials Conference, Baltimore, MD, June 1996.

(vii) U. Landman has been appointed as the director of a Nato Advanced Research Workshop on "Nanowires", Madrid, Spain, September 1996.

(viii) U. Landman has been elected as the chairman of the 10<sup>th</sup> International Symposium on Small Particles and Inorganic Clusters, to be held in Atlanta, August 2000.